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SOFTWARE RELEASE NOTES
FOR
PERIODIC UPDATE OF MODELS-3 SOFTWARE
(VERSION 2.3)

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EXHIBITS

1.0 INTRODUCTION

The U.S. Environmental Protection Agency (EPA) is empowered by current legislation to address today's important, grand challenge environmental problems, such as air quality management and linked air and water quality management. The use of environmental models is essential to EPA's cost effective accomplishment of its mission. As part of its High Performance Computing and Communications (HPCC) program, the Agency has initiated the development of a third-generation air quality modeling system called Models-3. Models-3 directly supports the HPCC program goal of using emerging computing and communications technology to:

- Develop the Agency's capability to perform complex multi-pollutant and cross-media pollutant studies that are currently not feasible due to computational limitations.

- Build federal, state, and industrial capabilities to use advanced assessment tools directly responsive to the needs for environmental management.

- Position the Agency to more easily integrate emerging computing and communications technology into environmental assessment tools, ensuring the most reliable and timely response to key environmental issues.

The Models-3 project is one of several being developed under the HPCC program. In many respects, however, Models-3 is the primary focus of EPA's HPCC research activities in that all the other projects under HPCC are, in one way or another, going to make significant contributions to enhance the capabilities of the Models-3 system. The other projects include: 1) linkage of air and water quality models, 2) development and performance evaluation of numerical algorithms on parallel architectures for key environmental processes, 3) development of training and technology transfer approaches to provide state, federal, and industrial air quality scientists and decision makers with credible and useful air quality modeling and decision support tools, 4) implementation of advanced computing hardware, software, and network infrastructure to support HPCC research activities, 5) development of advanced collaboratory visualization and analysis techniques, and 6) outreach activities designed to introduce more EPA researchers to the benefits of HPCC technology in their own areas of interest.

Legal Authority: The High Performance Computing Act of 1991 authorized EPA to perform research directed toward incorporating advances in computing and communications technology into EPA's environmental assessment applications and transferring these advanced tools to key state, federal, and industrial users with decision-making responsibility.

Regulatory Authority: As mandated by Congress in the 1990 Clean Air Act Amendments, the states are required to use photochemical grid models, such as the Urban Airshed Model

(UAM) and the Regional Oxidant Model (ROM), to develop credible modeling demonstrations for attaining the National Ambient Air Quality Standards (NAAQS) as part of their State Implementation Plans.

Regional Acid Deposition Model (RADM) applications are required to support EPA client and policy offices, EPA regional offices, and the states in implementing mandates of the 1990 Clean Air Act Amendments, special agreements between states, and treaty obligations under the U.S. – Canada Air Quality Agreement and the U.N. Economic Commission for Europe.

1.1 Purpose

This document provides new information not appearing in other Models-3 documentation and discusses problems that have been discovered since the initial software release. Anyone having a problem with Models-3 should check this document first.

1.2 Scope

This document covers the Models-3 framework and any problems that may occur in getting to the individual models or tools used in the system. Problems with the models or tools themselves, however, are not covered in this document.

1.3 Identification

The sponsor of Models-3 is the National Exposure Research Laboratory (NERL) in EPA's Office of Research and Development. Work on Version 2.3 of Models-3 was performed under MOSES Delivery Order 0055-076. The product control number for this release is SDC-0055-076-KB-8007.

2.0 REFERENCES

Novak, J.H., R.L. Dennis, D.W. Byun, J.E. Pleim, K.J. Galluppi, C.J. Coats, S. Chall, & M.A. Vouk. *EPA Third Generation Air Quality Modeling System, Models-3 Volume 1: Concept.* EPA/600/R95/084, National Exposure Research Laboratory, Research Triangle Park, NC, 55 pp. (1995).

EPA Third Generation Air Quality Modeling System, Models-3 Volume 9a: System Installation and Operations Manual. EPA/600/R-98/069(a), National Exposure Research Laboratory, Research Triangle Park, NC, 131 pp. (1998).

EPA Third Generation Air Quality Modeling System, Models-3 Volume 9b: User Manual. EPA/600/R-98/069(b), National Exposure Research Laboratory, Research Triangle Park, NC, 833 pp. (1998).

EPA Third Generation Air Quality Modeling System, Models-3 Volume 9c: User Manual: Standard Tutorial. EPA/600/R-98/069(c), National Exposure Research Laboratory, Research Triangle Park, NC, xxx pp. (1998).

EPA Third Generation Air Quality Modeling System, Models-3 Volume 10: System Implementation and Maintenance. EPA/600/R98/136, National Exposure Research Laboratory, Research Triangle Park, NC, xxx pp. (1998).

3.0 SUMMARY OF FUNCTIONALITY

Models-3 is not a single model or modeling system but rather a problem-solving environment containing components that help the user build, evaluate, and apply air quality models. Each shaded item in Exhibit 1 represents a component that helps the user perform major functions associated with environmental modeling.

Models-3's Object Oriented Data Base Management System (OO DBMS) provides a centralized method for managing and sharing data, metadata (information about data), program and/or script executables, and relationships and dependencies among executables and data needed for a specific modeling study. Each of the Models-3 components communicates with the OO DBMS as shown in Exhibit 1. These components serve as user-friendly tools for accessing or modifying datasets and source codes, developing program or script executables, performing model simulations, and visualizing and analyzing model simulation results.

The major Models-3 framework components are described in the following sections.

3.1 Program Manager

Program Manager allows the user to register, update, and search for executable programs, scripts, or both, and make them available for use in defining studies within the Study Planner component. During program registration, the user enters into the framework the characteristics of the program, including descriptive information on program function, input requirements, output specifications, runtime environment variables, target host computer, and operating system. Once the program or script is registered, this executable can be used in Study Planner to sequence a series of executions that may depend on previous executions for input data. The user can access and execute programs that are not registered, but using registered programs benefits the user in two ways. First, it enables the user to ensure that all

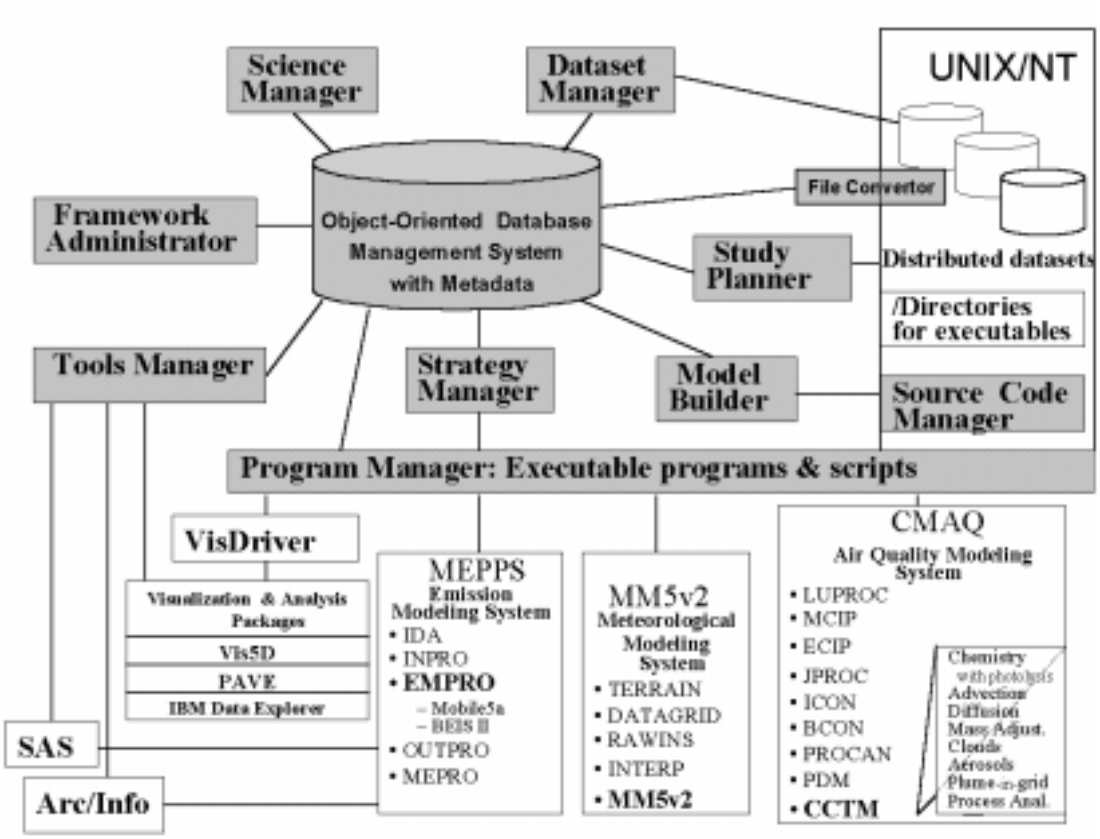

Exhibit 1. Models-3 Framework Components & Integrated Programs

mandatory inputs have been specified. Second, it automatically names and registers output files to facilitate tracking output from numerous program executions. Recommended model configurations for standard domains will be preregistered in the system, eliminating the need for the typical user to deal with program registration details.

3.2 Source Code Manager

Source Code Manager stores and retrieves source code for scientific models. It allows the user to retrieve a version of a source code file, change it, and return it to the code archive after the change has been tested. After a file has been returned to the archive, other users can access the updated version of the file. Source Code Manager tracks source code historical information and is used in the compilation process.

While the source code should not be changed for most user applications, the Community Multiscale Air Quality (CMAQ) model source code is included because it is needed for

recompilation with different user-specified grid domains. The source code is also needed for model development and testing, which often require source code modifications.

3.3 Science Manager

Science Manager allows the user to define globally-shared information on critical model components. In the past, details on horizontal grid coordinates, map projections, vertical layers, and chemical mechanisms have been hardwired and buried within most air quality model codes. In Models-3, details on these key science components are entered only once by the user from graphical user interfaces (GUI) controlled by the Science Manager. The specifications are then saved as named entities in an object-oriented data base accessible to all model components. In a typical application, a user would modify an existing set of specifications to define a new modeling domain.

More knowledgeable users might use Science Manager to experiment with new model components. To test alternative photochemical mechanisms, for example, the researcher would use Science Manager to edit one of the existing mechanisms, import a new set of chemical reactions, or specify new chemical species. Both Regional Acid Deposition Model - Version 2 (RADM-2) and Carbon Bond IV (CB-IV or CB-4) mechanisms are contained within this release of Models-3/CMAQ. If the chemical species for the new mechanism is present in the source emission profiles, then specifications for this new chemical mechanism would propagate to the emission processing subsystem, and an emission species would be generated consistent with the new chemical mechanism. Historically, testing a new chemical mechanism in this manner would have involved extensive error-prone software modifications. Science Manager reduces both the danger of software errors and the time needed to test alternative science components.

3.4 Model Builder

A typical user would access Model Builder to prepare a model for execution in a different location and/or to select an alternative horizontal/vertical grid resolution, and/or chemical mechanism, without the need for reprogramming. A model developer would use Model Builder to interchange science components within a model; modify details within an existing chemistry mechanism; or experiment with new horizontal and vertical resolutions, coordinate system, nested domain specifications, etc. Model Builder also assists with development of configuration files for creating new model executables from selected existing, modified, and new science process components.

3.5 File Converter

File Converter processes raw input data from American Standard Code for Information Interchange (ASCII) or Statistical Analysis System (SAS) files and converts it into formats

used in the Models-3 framework (Input/Output Application Programming Interface [I/O API] and SAS). The raw data should be delimited by spaces, tabs, or commas. File Converter can be accessed through the Tools Manager, through Dataset Manager if specific settings are made, or it can be used independently outside of the Models-3 framework. The most common use for File Converter is importing data, such as monitor data, into Models-3 to analyze or compare with model output using Models-3 visualization packages. File Converter can be used to import new input data for a model simulation, if the standard data files provided with this release are not suitable for the user's modeling needs. Models-3 also uses the File Converter to convert between internal data formats. This is an automatic process that the user does not direct.

3.6 Dataset Manager

Dataset Manager provides the user with the capability to register datasets for use with modeling and analysis programs in Models-3. The registration process involves entering the location of the dataset (full pathname) and metadata (information about the data, such as spatial–temporal extent and resolution, source of data, time convention, units, etc.) into the Models-3 data base. Models-3 follows the Federal Geospatial Metadata Standard for metadata content. The datasets may be located on any network-connected computer system known to the Models-3 system at the user's site. Once a dataset is registered, the user can search for the dataset based on its metadata information, file type, etc.

Dataset Manager allows the user to view the details of the selected dataset to ensure that the correct one has been selected for use with an application. Dataset registration eliminates the need for the user to type the entire pathname each time the dataset is used. Instead, the dataset can be highlighted from a list of candidates that satisfy the search criteria specified by the user. Models-3 will automatically move selected data to the host where it is needed for a model execution. Dataset Manager also provides standard capabilities like deleting, copying, archiving, and restoring files and metadata.

3.7 Strategy Manager

With Strategy Manager, the user can estimate future year point-, area-, and mobile-source emissions and determine the relative effectiveness of specified control scenarios. The user may adjust pollutant growth factors and emissions control factors to perform "what if" analyses for EPA regions, states, counties, or user-defined study areas. By applying estimated yearly emission growth factors from the Emissions Growth and Assessment System, and control efficiency, rule effectiveness, and rule penetration factors to EPA's 1990 base year emissions inventory, Strategy Manager estimates future year (1991–2010) emissions for carbon monoxide, nitrogen oxide, particulate matter up to 10 microns, sulfur dioxide, and volatile organic compounds. Strategy Manager is based on EPA's Multiple Projection

System. An input data processor will be added to process the Emission Inventory Improvement Program (**http://www.epa.gov/oar/oaqps/eiip**) data format after it is finalized.

3.8 Tools Manager

Tools Manager provides access to a variety of visualization, statistical analysis, and emissions processing tools that are registered with the Models-3 framework. The tools that are accessible are Vis5D, Text Editor, Models-3 Emission Processing and Projection System (MEPPS), Package for Analysis and Visualization of Environmental Data (PAVE), SAS, ARC/INFO, Inventory Data Analyzer (IDA), and VisDriver. MEPPS is an advanced tool that can be used for specifying emissions preparation and processing emissions details. MEPPS can also import emissions inventory data, perform quality control on emissions inventory data, and reformat or subset data for the user-specified modeling domain. Mobile emissions are calculated using Mobile 5a emission factors, and biogenic emissions are calculated using the Biogenic Emissions Inventory System (BEIS2). The system used in MEPPS for the main emissions processing requires the user to have ARC/INFO and SAS licenses for operation. These licenses are not included with Models-3.

3.9 Study Planner

Study Planner allows the user to define a study and control the execution of its associated models and processors. A study is a collection of plans and properties necessary to describe and perform one or more environmental modeling analyses. A plan is a collection of information defining dataset and program interdependencies. Study Planner gathers much of its information from the Program Manager and Dataset Manager registration data. The relationship between a program (node) and its required and optional datasets (links) is user-defined through the process of constructing and annotating a graphical diagram with simple drag-and-click mouse operations. Once a plan is constructed and its graphical diagram fully annotated with desired input datasets and options, the plan can be executed. User specified program options are entered by editing program environment variables.

Studies and associated plans are named entities that are saved in the system data base. Therefore, a typical user can start with an existing study plan provided by the model developer and simply change the dataset annotations by selecting, through a file browser, appropriate datasets needed for execution. The Study Planner provides the capability to create new studies, as well as copy, modify, and delete existing studies.

3.10 Framework Administrator

Framework Administrator allows the Models-3 framework administrator to register, update, and delete users, hosts, devices, compilers, and operating systems; establish access roles and

dataset types; and perform other administrative tasks. Refer to the Models-3 installation guide for information on the Framework Administrator component.

4.0 DEGREE OF FUNCTIONALITY PROVIDED

This section provides a list of software fixes since the last release, any assumptions or limitations of the Models-3 framework broken down by Models-3 component, any bugs found during testing of the released version, and any requirements that were only partially addressed in prior documentation.

4.1 Fixes Since Last Release

Several problems were uncovered after the last full release of the Model-3 framework have been corrected by the version 2.2a patch release.

- First, the File Migrator routines were changing the path of a file and affecting later operations. Second, files were not being copied properly to remote hosts due to the use of the wrong user ID. Third, files were also using the wrong user ID when verifying that the files existed. These problems have been fixed resulting in new versions of the following files: M3FM, M3SP, M3GI, and M3GI.vr.

- Some problems in the emissions portion of Models-3 were also discovered and have been corrected by this patch release. MEPPS grid and case creation through the Models-3 framework did not work. The problem has been corrected and affects the following files that now must be updated: makgridm.sas and makscenm.sas.

- A problem was found whereby the “MV Temporal Adjustment File Load” screen was not displaying correctly. The following files require updating to fix this problem: gemap.sct01 (Sun version), gemap.sc2 (NT version), and gemap.trans (Transport version).

- The landuse data base had a problem that caused improper values for three northeastern Mexican states. The landuse.dat file was updated with correct values and must be updated for this patch.

- In Models-3 Emissions Projections (MEPRO), there are Source Classification Codes (SCC) files necessary for changing the data base that were not included in the previous version. Although the files will be created the first time the data base is used, it will take many hours. We have included the SCC files required for the tutorial, and they will be copied to the same directory as the data base to keep the

program from having to create them. In the future, the SCC files will be created and distributed with all the data bases.

Some problems were discovered after the patch release of the Model-3 framework and have been corrected by the version 2.3 release. They include problems with the About box, the Dataset report and creating of directories on the NT.

4.2 Assumptions, Limitations, and Problems

The following paragraphs present some of the assumptions, limitations, and problems with various Models-3 components.

4.2.1 Presenter

This section addresses some common problems found in the graphical interface of the Models-3 framework. These problems either appear in several places at once or affect the application as a whole.

- If you have selected a remote host that has been registered as Orbix-enabled but Orbix is not running, problems can occur and the Models-3 framework may crash.

- The print function will not work properly in certain complex windows. The problem appears in the Galaxy libraries. No immediate action is planned to remedy the problem.

- Every object—such as dataset, program, etc.—has a unique ID that the user normally would not need to know. However, when uniqueness is required, the ID can assist the user in distinguishing among different objects with the same name. The user can reveal the IDs in both the summary and detail windows. Simply drag out the summary windows and an ID column will appear. In the detail windows, go to the menu bar, click the *View* menu item, and select *Hidden Info*. An informational pop-up window that includes the ID will appear.

- If the user exits while a save is in progress, an “object not saved” type of message appears. The user should select *Cancel* and wait to avoid any problems. If the object has been saved, a “saved successfully” type of message is displayed. If the user has saved an object but it has taken a while and no message has appeared, the object can be saved again.

- On rare occasions, the Orbix daemon may get suspended when it is started directly from UNIX. This is sometimes caused by Concurrent Versions System (CVS). The user should always use the m3run script to keep this from happening.

- When an object other that a dataset is copied, the server thinks it is editing the original object. If the original object is edited before the copy is saved, the message "Someone else is editing this object" will be displayed. The message can be ignored. After saving the object, the message will not appear again.

4.2.2 Dataset Manager

- Not all lists are sorted in the detail window.

- When copying an auto-registered dataset, the host and program name in the history entry is changed to a blank and Models-3, respectively.

- When selecting *Dataset/Visualize* at the menu bar of a DS detail screen, a Vis5D format file is expected. To use an IO/API format file, the VisDriver from the Tools Manager must be used.

- The *Dataset/Move* does not catch the error when the user specifies a file that is really the same file but different hosts were provided. (The file is mounted on both hosts.)

4.2.3 Study Planner

- When copying selected nodes, datasets, or both, with their connected edges from one plan to another, the edges are not correctly updated visibly on the screen when an individual node or dataset is moved. This is corrected after saving and refreshing the study.

- When clearing an environment variable that is a higher-level environment variable (i.e., a study or plan) from the Node Properties screen, the environment variable will not be displayed when going back into the Node Properties until some other action is done (e.g., pressing *Cancel* on the Node pop-up then coming back in).

4.2.4 Strategy Manager

There are no known problems in bringing up MEPRO from the framework.

4.2.5 Program Manager

The physical file is not deleted when delete is selected. This option now only deletes the metadata.

4.2.6 Science Manager

- If bad data is entered into the horizontal grid specifications that does not allow the grid to be viewed, an error message is displayed in the Orbix window, and the grid viewer will not be displayed.

- In the Vertical Layering detail window, you can generate the vertical layers as many times as you want. Once the metadata is saved, you cannot change the vertical layering type or regenerate the vertical layers. However, you can add to or otherwise modify the existing vertical layers.

- The user manual states that the Chemical Mechanism and the Configuration File Find screens have a selection field called “Created by.” Actually, the system allows a “Last modified by (user ID)” entry, so the Find screens were updated to reflect the correct operation.

- When copying a horizontal coordinate system, the projection parameters are not copied.

- When editing two horizontal coordinate systems at the same time, only one projection parameters pop-up window can be displayed at a time.

4.2.7 Model Builder

Model Builder was not implemented for the CRAY.

4.2.8 Tools Manager

There are no known problems.

4.2.9 Source Code Manager

The Source Code Manager button is disabled in this release. The user can still use CVS (distributed with this release) to perform source code management outside the framework.

4.2.10 Execution Manager

When executing nodes, a process is created called M3EMmon. Each node that is executed will leave one process. To remove these processes, the user should run M3EMkillMon.sh from the UNIX prompt only when no one is executing nodes on the machine. This procedure will only remove the M3EMmon processes that have no child processes (the ones that need to be removed). If a node is just starting or just ending execution, this script file may remove the wrong M3EMmon and cause the execution of nodes to stop on that node.

4.2.11 File Migrator

- For File Migrator to function best, there should be a “models3" user on any UNIX system. Also, the M3TEMP directory should be a mounted directory if using a machine other than the one the servers are loaded on.

- Remember that to function properly, the .rhosts file of each user of any non-Orbix enabled machine must allow access to the user and machine that is running the File Migrator. Please refer to the Models-3 *Volume 9a: System Installation and Operations Manual* for more instructions.

4.2.12 Help Server

- Help is displayed through an Internet browser. The user’s system must have a default browser installed to see Help. Also, the browser must take a command line argument. If the browser is already started, the system will not “un-iconize” it and bring it to the front. This may cause some confusion if the user does not remember when he/she “iconized” it, or when it is not visible.

- The Help buttons on the Node Properties and the Link Properties windows do not work. Select Help from the Study Planner detail windows and scroll down.

- *Index*, *Tutorial*, and *On Context* from the Help pull-down menu are not implemented.

4.2.13 Data Base

There are no known problems.

4.2.14 File Converter

When using free format and specifying a Fw.d format, the w (width) is ignored, and the display for a value less than 1 is 0.xx with d decimal accuracy.

4.2.15 IDA

There are no known problems.

5.0 INSTALLATION INSTRUCTIONS

Please refer to the Models-3 *Volume 9a: System Installation and Operations Manual* for installation instructions for Version 2.3.